# Stratified Turbulence in the Atmosphere and Oceans: A New Subgrid Model

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#### ABSTRACT

Turbulence in a stratified medium is studied with emphasis on stable stratification, as it occurs in the atmosphere and oceans, and on the construction of a subgrid model (SGS) for use in large eddy simulation (LES). The two basic assumptions of all SGS models are 1) that the unresolved scales are isotropic and 2) that they can be described by a Kolmogorov spectrum and are no longer valid in a stably stratified medium. Generation of gravity waves invalidates the second assumption, while the damping of vertical motion induces a degree of anisotropy considerably higher than in unstably stratified flows.

First, Weinstock's model is used to find that the energy dissipation rate  $\epsilon$  decreases with stability. By contrast, the dissipation rate  $\epsilon_{\theta}$  of temperature variance increases with stability. The effect of shear on the subgrid scales is neglected.

Second, because of the higher anisotropy of stably stratified flows, even the most complete SGS model presently in use must be enlarged to include new higher-order terms. A new second-order closure model is proposed in which the three components of the flux  $u_i\theta$  can be obtained by inverting a  $3\times 3$  matrix and  $\overline{u_i}u_j$  can be obtained by inverting a  $6\times 6$  matrix. An approximate procedure is suggested, however, to avoid the  $6\times 6$  matrix inversion and yet account for anisotropic production. The kinetic energy e is a solution of a differential equation. It is also shown that in a deep LES, where the buoyancy scales are fully resolved, the standard models for  $\epsilon$  and  $\epsilon_\theta$  are probably adequate, whereas in a shallow LES, where the buoyancy range may not be fully resolved, the above effects on  $\epsilon$  and  $\epsilon_\theta$  must be accounted for. It would be of interest to perform both a shallow and a deep LES so as to check the predictions of the model proposed here.

Preliminary results indicate that the (total) kinetic energy dissipation length scale increase with stability, in accordance with LES results but in disagreement with Deardorff's model that suggested a decrease of all dissipation scales in presence of stratification.

# 1. Introduction

At present, the most promising approach to study high Reynolds number turbulence is large-eddy simulation (LES), in which the largest energy-containing scales are fully resolved, while the unresolved subgrid scales must be represented via a subgrid scale (SGS) model (Wyngaard 1984; Galperin 1992).

Following Deardorff (1974) and Schumann (1991), we assume that the SGS functions needed in an LES, namely,  $b_{ij} = \overline{u_i u_j} - 2e\delta_{ij}/3$ ,  $\overline{u_i \theta}$  and e, are given by a second-order closure (SOC) model (an overbar indicates average over the grid size, whereas a tilde will be used to indicate ensemble average). The turbulent kinetic energy e satisfies a differential equation, while the differential equations for  $b_{ij}$  and  $\overline{u_i \theta}$  are usually converted to algebraic equations by neglecting the time derivative and the third-order moments. In principle, one can solve the resulting nine algebraic equations

and express analytically the tensor  $b_{ij}$  and the vector  $\overline{u_i\theta}$  in terms of the kinetic energy e, the mean shear S, and the mean temperature gradients  $\partial T/\partial x_i$ ; the latter are resolved quantities. Such a complete solution, however, has never been attempted. There are reasons for that. Physically, the unresolved scales are assumed to be considerably more isotropic than the resolved scales, and one can invoke a perturbative approach in the "smallness parameter"  $b_{ij}$  representing the departure from isotropy and classify the terms appearing in the equations for  $b_{ij}$  and  $\overline{u_i\theta}$  in terms of  $O(b^n)$ (Schemm and Lipps 1976). The most complete SGS model presently in use is the one suggested by Schmidt and Schumann (1989, referred to as SSM). In the equations for  $b_{ij}$ , they retain two terms of order O(1)and one term of order O(b), while the term representing anisotropic production, also of order O(b), is neglected. In the equation for  $u_i\theta$ , the authors retain only terms of order O(1), while neglecting two terms of order O(b).

The perturbative expansion in  $O(b^n)$  becomes less justified in the case of stable stratification as the turbulence is considerably more anisotropic due to the strong damping of the dynamical modes working against gravity. The safest approach would be to retain all the terms in the equations for  $b_{ij}$  and  $u_i\theta$ . This is

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easily accomplished for  $\overline{u_i\theta}$ , as all that is required is the inversion of a 3 × 3 matrix. The inversion of the 6 × 6 matrix needed to obtain  $b_{ij}$  is more complicated. Although the inversion can be implemented in a LES (M. Ypma, personal communication; see also Schmidt 1988), we also suggest a simplified procedure that leads directly to an expression for  $b_{ij}$  without matrix inversion

The extension of the model for  $b_{ij}$  and  $u_i\theta$  to include anisotropic effects is, in some ways, the easiest part of the problem. A major difficulty that has confronted all SGS models, especially when dealing with stably stratified flows, is the modeling of the dissipation rates of kinetic energy and temperature variance,  $\epsilon$  and  $\epsilon_{\theta}$ . In constructing these functions, it is assumed (e.g., see SSM) that the subgrid scales can be described by a Kolmogorov inertial spectrum (Ko is the Kolomogorov constant)

$$E(k) = \text{Ko}\epsilon^{2/3}k^{-5/3},$$
 (1)

which yields the well-known relation  $\epsilon \sim e^{3/2} l^{-1}$ , where  $l \approx \Delta$  is the kinetic energy dissipation length scale and  $\Delta$  is the size of the smallest resolved scale. Assuming (1) is physically equivalent to assuming (Turner 1973) that the subgrid scales do not undergo a transfer of energy directly to or out of them; that is, they only transfer energy from the largest scales to the smaller scales via nonlinear interactions. In this picture of "passive" eddies, the spectrum E(k) can depend only on the constant rate of energy transfer  $\epsilon$  and the local wavenumber k. In the case of stable stratification, the above picture is no longer valid since the eddies working against the stable stratification, that is, gravity, lose kinetic energy, which appears as potential energy represented by the  $(\delta \rho/\rho)^2$  fluctuations. This alone invalidates one of the basic assumptions on which Eq. (1) rests. The dissipation rate  $\epsilon$  no longer need enter the form of E(k). Instead, the physically relevant parameter is now the Brunt-Väisälä frequency N. With N and k, dimensional analysis demands that

$$E(k) \sim N^2 k^{-3},\tag{2}$$

which is the form of the energy spectrum suggested by Lumley (1964). The reason why the dissipation rate does not appear in (2) is because  $\epsilon$ , the residual energy that is ultimately transformed into heat, is not representative of the spectral region where the transformation of kinetic to potential energy takes place. Because of the loss of kinetic energy, the actual energy that is left to be dissipated into heat must be considerably less than the physical transfer  $\epsilon(k)$  that occurs in the spectral range described by (2). As much as kinematic viscosity does not enter the Kolmogorov spectrum but serves to define its region of validity, so is the role of  $\epsilon$  in this case. It enters the definition of the wavenumber  $k_0$  such that for  $k < k_0$  Eq. (2) holds while for  $k > k_0$ , we have Eq. (1). With N and  $\epsilon$ ,  $k_0 = (N^3 \epsilon^{-1})^{1/2}$ , which is often

referred to as the Ozmidov wavenumber. Lumley's expression for E(k) has the form

$$E(k) = \text{Ko}\epsilon^{2/3}[1 + (k/k_0)^{-4/3}]k^{-5/3}, \quad (3)$$

and this encompasses both spectral regions (1) and (2), referred to as the *inertial and buoyancy subranges*, respectively.

Even from this simplified discussion, it is clear that if one computes the kinetic energy e of the subgrid scales

$$e = \int_{\pi/\Lambda}^{\infty} E(k) dk \tag{4}$$

using Eq. (1), one finds the well-known  $\epsilon - e$  relationship,

$$\epsilon = c_{\epsilon}e^{3/2}/\Delta, \quad c_{\epsilon} = \pi \left(\frac{2}{3\text{Ko}}\right)^{3/2}.$$
 (5a)

This model has been used with success in several LES calculations of neutral and unstably stratified flows. In the case of stably stratified flows, use of (3) in (4) still leads to the functional form (5a). Instead of the constant  $c_{\epsilon}$ , however, one has an energy-dependent  $C_{\epsilon}(e)$  given by

$$C_{\epsilon}(e) = c_{\epsilon} \left(1 - \frac{1}{2} \operatorname{Ko} \pi^{-2} \frac{\Delta^{2}}{\Delta_{B}^{2}}\right)^{3/2},$$
 (5b)

where  $\Delta_B$  is a buoyancy length scale defined as

$$\Delta_B = \frac{e^{1/2}}{N} \,. \tag{5c}$$

Clearly, the applicability of the model is limited to  $\Delta < \pi \Delta_B (2/\text{Ko})^{1/2}$ . A significant improvement of Lumley's original model was proposed by Weinstock (1978, 1980, 1985, 1990), who pointed out, among other things, that a physically complete treatment of a stably stratified flow must account explicitly for the gravity waves that ultimately store the kinetic energy lost by the eddies, and that the derivation of (3) was based on an unjustified identification of Eulerian and Lagrangian time scales. This in turn implies that E(k) depends not only on N and k but also on the kinetic energy itself. In this case, the complete form of the spectrum

$$E(k, N, e) (5d)$$

is considerably more complex than Eq. (3); see Eqs. (B.6), and (B.9). In this paper, we adopt Weinstock's model to compute the general forms of  $C_{\epsilon}(e)$  and  $C_{\theta}(e)$ .

The organization of the paper is as follows. In section  $\underline{2}$ , we present the general expressions for e,  $b_{ij}$ , and  $\overline{u_i\theta}$  needed in an LES: the final results are expressed by Eqs. (6), (11), and (12). In section 3, we compute the functions  $C_{\epsilon}(e)$  and  $C_{\theta}(e)$  and thus the time scales  $\tau_{\epsilon}$  and  $\tau_{\theta}$ . In section 4, we present some conclusions and discuss plans for future research.

# 2. The expressions for e, $\overline{\theta^2}$ , $b_{ij}$ , and $\overline{u_i\theta}$

Since the derivation of second-order closure SOC models to construct the expressions for  $b_{ij}$  and  $\overline{u_i\theta}$  follows standard procedures, we shall quote here only the final results (see appendix A for details).

kinetic energy equation:

$$\frac{D}{Dt}e = -b_{ij}S_{ij} - \frac{\partial}{\partial x_i}\left(\frac{1}{2}\overline{q^2u_i} + \overline{pu_i}\right) + \lambda_i\overline{u_i\theta} - \epsilon$$
(6a)

equation for the temperature variance  $\overline{\theta^2}$ :

$$\frac{D}{Dt}\overline{\theta^2} = -2\overline{u_i}\overline{\theta}\frac{\partial T}{\partial x_i} - \frac{\partial}{\partial x_i}\overline{u_i}\overline{\theta^2} - 2\epsilon_{\theta} \qquad (6b)$$

equation for  $b_{ii}$ :

$$2c_4\tau_{\epsilon}^{-1}b_{ij} = t_2(1-c_5)B_{ij} - \frac{4}{3}(1-\alpha_0)eS_{ij}$$
$$-t_1(1-2\alpha_1)\Sigma_{ij} - t_1(1-2\alpha_2)Z_{ij}$$
 (7)

equation for  $\overline{u_i\theta}$ :

$$2c_{6}\tau_{\epsilon}^{-1}\overline{u_{i}\theta} = -\left(t_{3}b_{ij} + \frac{2}{3}e\delta_{ij}\right)\frac{\partial T}{\partial x_{j}} - t_{1}(aS_{ij} + bR_{ij})\overline{u_{j}\theta} + t_{2}(1 - c_{7})\lambda_{i}\overline{\theta^{2}}, \quad (8)$$

where (the flags t's, which can assume the values 0, 1, will be discussed shortly)

$$b_{ij} = \overline{u_i u_j} - \frac{2}{3} e \delta_{ij}, \quad \frac{1}{2} \overline{u_i u_i} = e,$$

$$\lambda_i = g_i \alpha, \quad g_i = (0, 0, g),$$

$$B_{ij} = \lambda_i \overline{u_j \theta} + \lambda_j \overline{u_i \theta} - \frac{2}{3} \delta_{ij} \lambda_k \overline{u_k \theta}$$

$$\Sigma_{ij} \equiv S_{ik} b_{kj} + S_{jk} b_{ik} - \frac{2}{3} \delta_{ij} S_{kl} b_{kl}$$

$$Z_{ij} \equiv R_{ik} b_{kj} + R_{jk} b_{ik} - \frac{2}{3} \delta_{ij} R_{lk} b_{kl}$$

$$2S_{ii} = U_{i,i} + U_{i,i}, \quad 2R_{ij} = U_{i,j} - U_{i,i}. \quad (9)$$

The constants a, b, and c will be discussed later. We note that the last term in  $Z_{ij}$  is always identically zero, for it is the product of a symmetric tensor and an antisymmetric tensor: it is included only to exhibit the symmetry with the term in  $\Sigma_{ij}$ .

As one can see, the equations for e,  $b_{ij}$ , and  $\overline{u_i\theta}$  require the knowledge of the dissipation rate  $\epsilon$  and the two time scales

$$\tau_{\epsilon} = \frac{2e}{\epsilon}, \quad \tau_{\theta} = \frac{\overline{\theta^2}}{\epsilon_{\theta}}, \quad (10)$$

which we will consider in the next section. Here, we shall discuss first Eqs. (7)-(8).

As for the equation for  $u_i \bar{\theta}$ , Eq. (8) can be written more compactly as

$$A_{ij}\overline{u_{i}\theta} = -\left(t_{3}b_{ij} + \frac{2}{3}e\delta_{ij}\right)\frac{\partial T}{\partial x_{i}} + t_{2}(1-c_{7})\lambda_{i}\overline{\theta^{2}}, (11a)$$

where

$$A_{ij} = 2 c_6 \tau_{\epsilon}^{-1} \delta_{ij} + t_1 (aS_{ij} + bR_{ij}).$$
 (11b)

Therefore, to obtain  $\overline{u_i\theta}$ , one needs to invert a 3 × 3 matrix.

In analogy with Schmidt (1988), we introduce the flags  $t_1$ ,  $t_2$ , and  $t_3$  to help classify the various model that have been used in the literature, namely:

- a) First-order closure, FOC:  $t_1 = t_2 = t_3 = 0$ ; these models are discussed in appendix A.
- b) Second-order closure, SOC2:  $t_1 = t_3 = 0$ ,  $t_2 = 1$ ; this model has been used by Schmidt (1988) and Schumann (1991).
  - c) Second-order closure SOC3:  $t_1 = 0$ ,  $t_2 = t_3 = 1$ .
  - d) Second-order closure, SOC1:  $t_1 = t_2 = t_3 = 1$ .

The most appropriate model to treat stably stratified flows and their inherent degree of anisotropy is the SOC1. In its complete form, a significant complication arises from the last two terms in Eq. (7) since they depend on  $b_{ij}$  itself, Eq. (9). While the inversion of the ensuing  $6 \times 6$  matrix is in principle feasible, Schmidt (1988) has discussed the difficulties that this procedure would entail. In light of his discussion, we suggest a simplified procedure whereby for the  $b_{ij}$  entering  $\Sigma_{ij}$  and  $Z_{ij}$  one may take the solution of (7) without the last two terms, in which case (7) becomes

$$2c_{4}\tau_{\epsilon}^{-1}b_{ij} = (1 - c_{5})B_{ij} - \frac{4}{3}(1 - \alpha_{0})eS_{ij}$$
$$- (1 - 2\alpha_{1})\Sigma_{ij}(b_{ij}^{0}) - (1 - 2\alpha_{2})Z_{ij}(b_{ij}^{0}) \quad (12a)^{2}$$
$$2c_{4}\tau_{\epsilon}^{-1}b_{ij}^{0} = (1 - c_{5})B_{ij} - \frac{4}{5}(1 - \alpha_{0})eS_{ij}. \quad (12b)^{2}$$

In Eq. (12a), the form of the tensors  $\Sigma_{ij}$  and  $Z_{ij}$  is still given by Eq. (9) but with  $b_{ij}$  substituted with the form of  $b_{ij}^0$  given by Eq. (12b). This approximate procedure avoids entirely the need to solve the  $6 \times 6$  matrix since the right-hand side of (12a), with the help of (11), is now expressed entirely in terms of the kinetic energy e and of the variables derivable from the LES.

In order to put the new model in perspective, we note that the most complete SGS model to date is the SOC2 model of Schmidt and Schumann (1989), represented by

$$2c_4\tau_{\epsilon}^{-1}b_{ij}=(1-c_5)B_{ij}-\frac{4}{3}(1-\alpha_0)eS_{ij}$$
 (13a)

$$2c_6\tau_{\epsilon}^{-1}\overline{u_i\theta} = -\frac{2}{3}e\frac{\partial T}{\partial x_i} - (1-c_7)\tau_{\theta}\lambda_i\overline{u_j\theta}\frac{\partial T}{\partial x_j}, (13b)$$

which implies that Eq. (6b) is considered in the sta-

tionary case and without the third-order moment. In Eq. (13a), the contribution from the anisotropic terms  $\Sigma_{ij}$  and  $Z_{ij}$  are neglected, and in (13b) the anisotropic term appearing in the first term of (8) is also neglected. If (13b) were to be regarded as an ensemble-average equation, it would imply that

$$\widetilde{u\theta} = 0, \tag{14}$$

whereas the data show  $u\theta \neq 0$ . It is also clear that the inclusion of the term  $b_{ij}\partial T/\partial x_j$  alone would already remedy this fact and make the model at least in qualitative agreement with the data. That is why we propose that SOC2 must be extended to at least SOC3 or, more completely, to SOC1.

In summary, we suggest that the SGS model for e,  $\theta^2$ ,  $b_{ij}$  and  $u_i\theta$  be given by Eqs. (6), (11), and (12) in the SOC1 version. The model still requires the funtions  $\epsilon$ ,  $\tau_{\epsilon}$ , and  $\tau_{\theta}$ , to which we now turn.

# 3. Dissipation in the presence of stratification: The Lumley-Weinstock model and the inclusion of gravity waves

The knowledge of  $\tau_{\epsilon}$  and  $\tau_{\theta}$  requires the knowledge of the dissipation rates  $\epsilon$  and  $\epsilon_{\theta}$ , Eq. (10). In determining  $\epsilon$  and  $\epsilon_{\theta}$  it is customary to write an expression of the form

$$\epsilon \sim \frac{e^{3/2}}{I},$$
 (15)

where l is some typical dissipation length. Since thus far it has always been assumed that the subgrid scales are inertial, l was chosen to be given by  $\Delta$  within a numerical constant. In the presence of stratification, the choice of the proper l is no longer so straightforward since in addition to  $\Delta$  one has the buoyancy scale  $\Delta_B$  defined in (5c), which could also be used in (15); however, since in an LES,  $\Delta$  is a well-defined quantity, we shall use it as the proper scale, thus writing  $\epsilon$  and  $\epsilon_\theta$  in the following form

$$\epsilon = C_{\epsilon}(e) \frac{e^{3/2}}{\Delta}, \quad \epsilon_{\theta} = \frac{1}{2} C_{\theta}(e) \overline{\theta^2} \frac{e^{1/2}}{\Delta}$$
(16)

so that

$$\tau_{\epsilon} = \frac{2}{C_{\epsilon}(e)} \frac{\Delta}{e^{1/2}}, \quad \tau_{\theta} = \frac{2}{C_{\theta}(e)} \frac{\Delta}{e^{1/2}}. \quad (17)$$

We shall now discuss the general expression for  $C_{\epsilon}$  and  $C_{\theta}$ .

# a. Unstable stratification

In this case, one can safely assume that the SGS do in fact "passively" transfer the energy from the large scales to the smaller scales without altering the net amount of energy involved in the process. Under these assumptions, the kinetic energy and temperature variance spectra are well represented by the inertial Kolmogorov and Obukhov forms,

$$E(k) = \text{Ko}\epsilon^{2/3}k^{-5/3}$$
  $G(k) = \text{Ba}\epsilon_{\theta}\epsilon^{-1/3}k^{-5/3}$ , (18)

where Ko and Ba are the Kolmogorov and Batchelor constants. When these spectra are used in the expressions for the subgrid kinetic energy Eq. (4) and temperature variance

$$\overline{\theta^2} = \int_{\pi/\Delta}^{\infty} G(k) dk, \tag{19}$$

one indeed obtains the expressions for  $\epsilon$  and  $\epsilon_{\theta}$  given by (16) with

$$C_{\epsilon}(e) \rightarrow c_{\epsilon} = \pi \left(\frac{2}{3 \text{ Ko}}\right)^{3/2},$$

$$C_{\theta}(e) \rightarrow c_{\theta} = \frac{4\pi}{3 \text{ Ba}} \left(\frac{2}{3 \text{ Ko}}\right)^{1/2};$$
(20)

that is, the functions C are constants related to the Kolmogorov and Batchelor constants and are therefore known (SSM, appendix B).

# b. Stable stratification: The effect of gravity waves

In the case of stable stratification, the physical arguments presented in section 2 indicate that we can no longer assume that (18) represent the subgrid scales since the spectrum exhibits two ranges, a buoyancy subrange and an inertial subrange. Equations (18) are valid only in the latter. In the buoyancy subrange the energy flow from the largest to the smallest scales under the action of nonlinearity is no longer the only process. Working against gravity, the eddies lose a fraction of their kinetic energy, which is transformed into potential energy represented by the  $(\delta \rho/\rho)^2$  fluctuations. This can be seen from Eqs. (6a) and (6b) where, in the case of stable stratification, the negative flux  $\overline{u_i\theta}$  acts as a source for  $\theta^2$  and a sink for the kinetic energy. The fraction of kinetic energy transformed into potential energy does not, however, simply cascade toward smaller scales under the action of an alternative dissipation mechanism (thermal conduction in the case of temperature). In fact, the latter is too inefficient to dissipate all the energy extracted from the eddies; the only alternative route is a backward flow toward larger scales (Schumann 1987; Dalaudier and Sidi 1987).

If  $\epsilon(k)$  and  $\epsilon_{\theta}(k)$  represent the fluxes of kinetic energy and temperature fluctuations across a given wavenumber k, we see from Fig. 1 that the inertial subrange defined by  $\epsilon(k) = \text{const} = \epsilon$  attains only for wavenumbers  $k \ge k_B$ , whereas for  $k \le k_B$ ,  $\epsilon(k)$  decreases with increasing k, indicating a net loss of energy from the eddies. In Figs. 2-4 we show the kinetic energy spectrum E(k), the temperature variance spectrum G(k), and the buoyancy spectrum B(k).

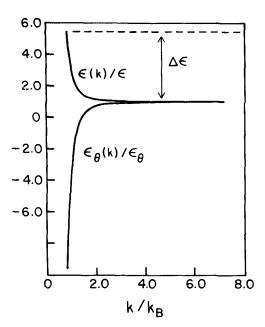


FIG. 1. Turbulent kinetic and mean-square temperature fluctuations spectral fluxes  $\epsilon(k)$  and  $\epsilon_{\ell}(k)$ , normalized to their constant values at  $k \to \infty$ . The wavenumber k is in units of  $k_B = (6/5)^{1/2} \mathrm{Ne}^{-1/2}$ , Eq. (B.7). Were it not for the emission of gravity waves,  $\epsilon(k)$  would become constant at a much smaller k,  $\epsilon(k) = \epsilon$  = constant indicated by the dashed line. The lowering of  $\epsilon(k)$  by  $\Delta \epsilon$  is discussed in the text; see Eqs. (21).

As one can note, the wavenumber  $k_B$  thus separates the two subranges: the buoyancy subrange containing gravity waves that are only weakly damped (and thus their effect is maximized), and the inertial subrange,

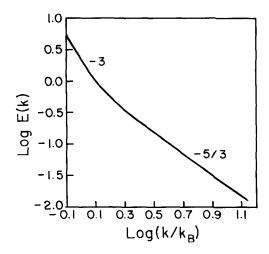


FIG. 2. Plot of the turbulent energy spectrum E(k), Eqs. (B.6) and (B.9), vs k, in units of  $k_B$  defined in Eq. (B.7). The Kolmogorov inertial range, denoted by the slope -5/3, is seen to attain at values of  $k \ge 2k_B$ . At lower values of k, the emission of gravity waves, with the corresponding loss of kinetic energy by the eddies, is reflected in the steeper slope of the order of -3. The latter is in accordance with recent direct numerical simulation results of Gerz and Schumann (1991, Fig. 5a) and with observational data (Weinstock 1978, 1985b; Gargett 1989, 1990).

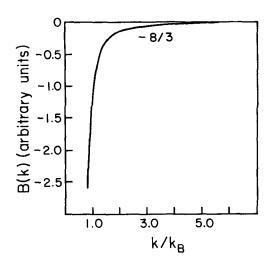


FIG. 3. The spectrum of the temperature flux  $\overline{w\theta}$ , B(k), Eq. (B.5) vs k in units of  $k_B$ ; see Fig. 1. As expected, the flux is negative and its steep variation with k near  $k_B$  is in accordance with the DNS results of Gerz and Schumann (1991, Fig. 7b).

where the gravity waves are strongly damped and in which there is a constant flux of energy,  $\epsilon(k) = \text{const} = \epsilon$ . One can alternatively view the new buoyancy subrange as a "buoyancy-modified turbulence," or as "turbulence-modified waves" since, as Gargett et al. (1981) have pointed out, one is dealing with "vertical scales between wavelike motion at larger scales and locally isotropic turbulence at smaller scales."

If no gravity waves were emitted by the eddies,  $\epsilon(k)$  would become constant at a smaller value of k (dashed line in Fig. 1), indicating a flux independent of wavenumber. In the present case, however, the physical dis-

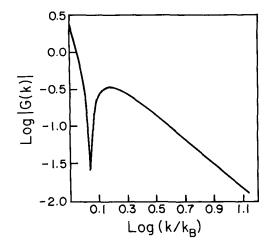


FIG. 4. The spectrum of the temperature variance G(k), Eqs. (18)–(19), vs k in the same units as in Fig. 1. The cusp is due to the fact that we have plotted the absolute value of G(k), which for  $k \le k_B$  is actually negative since there is a backward flow of potential energy from small to large scales (Dalaudier and Sidi 1987). See also Fig. 5b of Gerz and Schumann (1991).

sipation  $\epsilon = \epsilon(k = \infty)$  is far smaller. This can be seen from Eq. (A.9), which represents the conservation of kinetic plus potential energy. In the stationary case and neglecting third-order terms we have, with  $\Pi = -b_{ij}S_{ij}$ ,

$$\Pi = \epsilon + \frac{(g\alpha)^2}{N^2} \, \epsilon_{\theta}. \tag{21a}$$

Since in the unstable case,  $N^2 < 0$ , we have for constant II (the subscripts s and u stand for stable and unstable, respectively).

$$\epsilon^{s} = \epsilon^{u} - (g\alpha)^{2} |N^{2}|^{-1} (\epsilon^{s}_{\theta} + \epsilon^{u}_{\theta}); \qquad (21b)$$

Eq. (21b) thus implies that

$$\epsilon(\text{stable}) < \epsilon(\text{unstable})$$
 (21c)

as we set out to prove.

The first to present a heuristic model for these effects were Bolgiano (1959, 1962), Shur (1962), and Lumley (1964; for a review see Phillips 1965). As Phillips pointed out, there are difficulties with Bolgiano's model, so we shall discuss only the Shur-Lumley models. The first assumption was that the Kolmogorov form for the energy spectrum Eq. (18), which is valid under the assumption of constant energy flux  $\epsilon(k) = \text{const}$ , can be applied even when  $\epsilon$  is a function of k provided that

$$\left| \frac{k}{\epsilon} \frac{\partial \epsilon}{\partial k} \right| \ll 1. \tag{22}$$

The second assumption was that the separation wavenumber is taken to be  $k_0$ , which is a function of  $\epsilon$  and N only. Under these assumptions, Lumley's final result for the energy spectrum is Eq. (3), which predicts a unique  $k^{-3}$  spectrum in the buoyancy subrange. While atmospheric and oceanographic data (Gargett et al. 1981; Weinstock 1978, 1985; Dalaudier and Sidi 1987) are in qualitative agreement with this prediction, they actually show spectra ranging from -2.5 to -3. Moreover, in the buoyancy subrange where  $E(k) \sim k^{-3}$ condition (22) is not satisfied. More fundamentally, Weinstock (1978) pointed out that the main assumption that E(k) depends on  $\epsilon$  and k only [already questioned by Phillips (1965)] was actually not valid: the flux of kinetic energy must also depend on the kinetic energy of the eddies. Weinstock (1978) then proceeded to include explicitly the effect of gravity waves on the turbulent energy spectrum, thus achieving a more complete physical picture (appendix B). The derivation of the functions C is rather laborious and we shall quote here only the final results:

$$C_{\epsilon}(e) = c_{\epsilon} \exp(-0.053x^2)$$
 (23a)

$$x \equiv \frac{N\Delta}{e^{1/2}} = \frac{\Delta}{\Delta_B} \,. \tag{23b}$$

The function  $C_{\epsilon}$  versus  $\Delta/\Delta_B$  is shown in Fig. 5, where

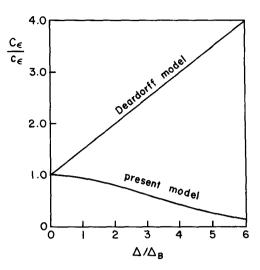


Fig. 5. The function  $C_{\epsilon}(e)/c_{\epsilon}$  entering the dissipation  $\epsilon$ , Eq. (16), as a function of  $\Delta/\Delta_B$ . As one can observe, the present model predicts a behavior in contradiction with Deardorff's model (1980). See Eq. (C.10) and Conclusions.

we also plot Deardorff's model (1980) for  $C_{\epsilon}$ , given by Eq. (C.10); namely;

$$C_{\epsilon}(e) = c_{\epsilon}^* \left( 1 + \frac{1}{2} \frac{\Delta}{\Delta_B} \right),$$
 (23c)

where  $c_{\epsilon}^* = 0.5$ . As one can see, the two models predict opposite behavior for  $C_{\epsilon}$ . Here we note the following.

#### 1) FINE-RESOLUTION LES

If one carries out an LES that resolves scales  $\Delta$  smaller than the buoyancy scale, that is, if  $\Delta/\Delta_B \leq 1$ , one has automatically included the buoyancy range into the LES, and therefore it can be assumed that the unresolved scales fall into the inertial range for which (20) hold true. Our model confirms this expectation; see Fig. 5. Stated differently, since in a deep LES one has actually succeeded in resolving almost all the relevant scales, one can reasonably expect that conclusions derived from a DNS be to some extent applicable. For example, Schumann (1991) has concluded that within a DNS, stratification does not greatly affect the dissipation length scale, meaning that one can take  $C_{\epsilon} \approx c_{\epsilon}$ , a result confirmed by our model; see Fig. 5.

# 2) Coarse-resolution LES

If the LES does not resolve the buoyancy range, that is, if  $\Delta/\Delta_B \ge 1$ , the subgrid scales are not fully inertial and the effect of stratification must be accounted for since  $C_{\epsilon}$  may be significantly different than  $c_{\epsilon}$ . This expectation is indeed borne out by Fig. 5, where  $C_{\epsilon}$  becomes considerably smaller than  $c_{\epsilon}$ , indicating the physical fact that in this case one has less dissipation since, as discussed earlier, the eddies have emitted a

fraction of their energy in gravity waves thus leaving behind less energy to be dissipated.

One must therefore conclude that the new physical phenomenon described by  $C_{\epsilon}(e)$  may or may not be relevant to an LES calculation depending on how deep the resolution is.

As for  $C_{\theta}(e)$ , the model predicts the following results:

$$C_{\theta}(e) = C_{\epsilon}(e)\omega^{-1} \left[ \frac{c_{\theta}}{c_{\epsilon}} - 2\gamma(\omega - 1) \frac{e}{\theta^{2}} \right]$$
 (24a)

$$\omega(e) \equiv \exp(-0.053 x^2), \quad \gamma \equiv N^{-2} |\nabla T|^2, \quad (24b)$$

where both e and  $\overline{\theta^2}$  are still in general time dependent. Some considerations are in order. Physically, one expects that in a *fine-resolution LES*,  $x \le 1$ , both  $C_{\epsilon}$  and  $C_{\theta}$  be almost stratification independent; for this to be so,  $\omega$  must be of order unity, which Eq. (24b) confirms to be the case.

On the other hand, in the case of a coarse-resolution LES,  $x \ge 1$ , the decrease of kinetic energy dissipation  $\epsilon$ , represented by  $C_{\epsilon}/c_{\epsilon} < 1$ , must be compensated by an increase in dissipation of temperature variance, which implies that

$$C_{\theta}(e)/c_{\theta} > 1. \tag{25}$$

The SGS model is now complete. One must solve Eqs. (6), (11), and (12) in conjunction with (17), (23a,b), and (24). Much as the choice of the appropriate  $C_{\epsilon}$  and  $C_{\theta}$  depends on the nature of the LES (deep or shallow), so does the choice of the SOC model. For example, in the case of a deep LES, one may argue that the anisotropic contributions to  $b_{ij}$  and  $\overline{u_i\theta}$  may be less important than in the shallow LES case and thus one may resort to an SOC2; in a shallow LES approach, however, it seems inevitable that one must use the full SOC1. Finally, it is clear that the need to account for three spatial dimensions does not allow the introduction of simple parameterization of  $\overline{u_i\theta}$  and  $b_{ij}$  in terms of diffusion length scales of heat and momentum.

### 4. Conclusions

The search for an SGS model for LES calculations is a difficult and challenging problem, for it involves the heart of turbulence: the dynamics of the high vorticity small scales. If one could assume that these scales satisfy Kolmogorov's strict conditions of being passive "transferers" of energy from the larger to the smaller scales, the problem would be solvable. The assumption of "inertiality" of the subgrid scales is probably reasonable in the case of unstable stratification, but it ceases to be so in the case of stable stratification, where gravity removes kinetic energy from the eddies: the generation of gravity waves becomes the dominant physical process, with dissipation relegated to higher wavenumbers. The loss of kinetic energy favors the creation and maintenance of fluctuations  $(\delta \rho/\rho)^2$ , which become an integral part of the overall dynamics. Equation (21a) expresses the fact that the total production  $\Pi$  is now dissipated by both  $\epsilon$  and  $\epsilon_{\theta}$ , in sharp contrast to the unstable case.

The main result is that

$$\epsilon$$
(stable) <  $\epsilon$ (unstable); (26)

that is, the loss of kinetic energy to create gravity waves leaves behind less energy to be dissipated by molecular processes. By the same token, the creation of  $(\delta \rho/\rho)^2$  fluctuations increases the amount of energy stored in potential form with the consequence that there is more left to dissipation; that is,

$$\epsilon_{\theta}(\text{unstable}) < \epsilon_{\theta}(\text{stable}).$$
 (27)

These two facts are represented mathematically by the functions  $C_{\ell}(e)$  and  $C_{\theta}(e)$ , which are

$$C_{\epsilon}(e)/c_{\epsilon} < 1, \quad C_{\theta}(e)/c_{\theta} > 1.$$
 (28)

Since the expressions for the C's have been derived without assuming a specific closure of the Navier-Stokes equations, they could, in principle, be used in any closure model. There is an interesting exception, however, the FOC model, as we shall now show.

In fact, using  $t_1 = t_2 = t_3 = 0$  in Eqs. (7)–(8) we obtain

$$b_{ij} = -c_1 e^{1/2} \Delta S_{ij} C_{\epsilon}^{-1} \tag{29}$$

$$\overline{u_i\theta} = -c_2 e^{1/2} \Delta \frac{\partial T}{\partial x_i} C_{\epsilon}^{-1} \equiv -l_h(\text{FOC}) e^{1/2} \frac{\partial T}{\partial x_i}$$
 (30)

$$\epsilon = g_i \alpha \overline{u_i \theta} - b_{ii} S_{ii}. \tag{31}$$

Substituting (29)–(30) into (31) we obtain an expression for the energy e; use of it in (30) finally gives the expression for the convective flux, ( $\sigma_t = c_1/2c_2$ )

$$\overline{u_i\theta} = -K_h(\text{FOC})\frac{\partial T}{\partial x_i}$$
 (32)

$$K_h(\text{FOC}) = c\Delta^2 S(1 - \text{Ri}\sigma_t^{-1})^{1/2} C_{\epsilon}^{-2}.$$
 (33)

If one takes

$$C_{\epsilon}(e) = c_{\epsilon}, \tag{34}$$

it is known that the convective fluxes given by (32) are too large. This shortcoming has traditionally been amended by adopting Deardorff's model (1980), whereby [see Eq. (C.10)]

$$C_{\epsilon}^{*}(e) = c_{\epsilon} \left( 1 + \frac{1}{2} x \right) \tag{35}$$

so that

$$C_{\epsilon}(e) > c_{\epsilon},$$
 (36)

thus lowering the flux. The main result of this paper, however, is that

$$C_{\epsilon}(e) < c_{\epsilon}.$$
 (37)

If one were to adopt the new model for  $C_{\epsilon}(e)$ , Eq. (32)

would yield even larger fluxes than in the  $C_{\epsilon}(e) = c_{\epsilon}$  case. This can only be construed as indicating a structural deficiency of the FOC model (32).

We suggest the SOC1 closure model, together with the new expressions for  $C_{\epsilon}(e)$  and  $C_{\theta}(e)$ , as a model that shows no internal inconsistencies and correctly describes the behavior of stably stratified flows.

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#### APPENDIX A

# The Second-Order Closure Model: SOC

Using the Reynolds stress formalism, one derives the following equations for  $b_{ij}$ ,  $\overline{u_i\theta}$ , and  $\theta^2$  (e.g., see Donaldson 1973; Zeman and Lumley 1976; Schemm and Lipps 1976; Lumley et al. 1978; Zeman 1981):

$$\frac{D}{Dt} b_{ij} = -\Sigma_{ij} - Z_{ij} + B_{ij} - \Pi_{ij} - D_{ij} - \frac{4}{3} eS_{ij} \quad (A.1)$$

$$\frac{D}{Dt}\overline{u_i\theta} = -\left(b_{ij} + \frac{2}{3}e\delta_{ij}\right)\frac{\partial T}{\partial x_j} - \overline{\theta u_j}\frac{\partial U_i}{\partial x_j} + \lambda_i\overline{\theta^2} - \Pi_i^{\theta} - \frac{\partial}{\partial x_i}\overline{\theta u_i u_j} \quad (A.2)$$

$$\frac{D}{Dt}\overline{\theta^2} = -2\overline{u_i}\overline{\theta}\,\frac{\partial T}{\partial x_i} - \frac{\partial}{\partial x_i}\,\overline{u_i}\overline{\theta^2} - 2\epsilon_{\theta},\quad (A.3)$$

where  $\lambda_i = g_i \alpha$  ( $\alpha$  is the volume expansion coefficient) and  $D/Dt = \partial/\partial t + U_j \partial/\partial x_j$ ;  $D_{ij}$  is the third-order moment defined as

$$D_{ij} = \frac{\partial}{\partial x_k} \left[ \overline{u_i u_j u_k} - \frac{1}{3} \delta_{ij} \overline{q^2 u_k} \right]. \tag{A.4}$$

Other symbols are defined in Eq. (9). The pressure correlations are defined by

$$\Pi_{i}^{\theta} \equiv \theta \frac{\partial p}{\partial x_{i}}, \quad \Pi_{ij} \equiv u_{i} \frac{\partial p}{\partial x_{j}} + u_{j} \frac{\partial p}{\partial x_{i}} - \frac{2}{3} \delta_{ij} \frac{\partial}{\partial x_{k}} \overline{pu_{k}},$$
(A.5)

and following Zeman and Lumley (1976, 1979) and Zeman (1981), we take

$$\Pi_{i}^{\theta} = 2c_{6}\tau^{-1}\overline{u_{i}\theta} + c_{7}\lambda_{i}\overline{\theta^{2}} + \frac{\partial}{\partial x_{i}}\overline{p\theta} 
- \frac{4}{5}a_{m}(S_{kj} + R_{kj}) \left[ \delta_{ik}\overline{\theta u_{j}} - \frac{1}{4}\delta_{ij}\overline{\theta u_{k}} \right] \quad (A.6)$$

$$\Pi_{ij} = 2c_{4}\tau^{-1}b_{ij} + c_{5}B_{ij} - \frac{4}{3}\alpha_{0}eS_{ij} - 2\alpha_{1}\Sigma_{ij} - 2\alpha_{2}Z_{ij}.$$
(A.7)

We may note that if  $2\alpha_1 = 2\alpha_2 = \alpha_0 \equiv \gamma$ , the sum of the last three terms in Eq. (A.7) coincides with the expression given by Rodi [1984, Eq. (2.64)].

Since the contraction Eq. (A.1) yields an identity, we must supplement the above equations with the dynamical equation for the turbulent kinetic energy e. This is Eq. (6a). Introducing the potential energy P (Dalaudier and Sidi 1987),

$$P = \frac{1}{2N^2} (g\alpha)^2 \overline{\theta^2}, \qquad (A.8)$$

the sum of the total fluctuating energy, kinetic plus potential,  $\underline{e} + P$ , satisfies the following equation,  $F_{KE}^i = 1/2q^2u_i + \overline{pu_i}$  is the generalized kinetic energy flux,

$$\frac{D}{Dt}(e+P) = -b_{ij}S_{ij} - \left[\epsilon + (g\alpha)^2 N^{-2}\epsilon_{\theta}\right] - \frac{\partial}{\partial x_i} \left[F_{KE}^i + \frac{1}{2}(g\alpha)^2 N^{-2}\overline{u_i\theta^2}\right]. \quad (A.9)$$

As expected, the convective flux,  $\overline{u_i\theta}$ , which physically represents a mechanism to convert kinetic into potential energy or vice versa, has disappeared from Eq. (A.9). Finally,  $\epsilon$  and  $\epsilon_{\theta}$  are the dissipation rates of energy and temperature fluctuations.

In the stationary case and neglecting the third-order moments, Eqs. (A:1)-(A.2) reduce to Eqs. (7)-(8) of the text, where  $a = 1 - 3a_m/5$  and  $b = 1 - a_m$ .

### APPENDIX B

# The Dissipation Rates $\epsilon$ and $\epsilon_{\theta}$

Following Phillips (1965), the kinetic energy spectrum E(k) and mean-square temperature fluctuation spectrum G(k) satisfy the following equations:

$$\frac{\partial E}{\partial t} + \frac{\partial Q_i}{\partial x_i} = -\frac{\partial \epsilon}{\partial k} - \beta_{ij} S_{ij} + \lambda_i B_i(k) - 2\nu k^2 E(k)$$
(B.1)

$$\frac{\partial G}{\partial t} + \frac{\partial H_i}{\partial x_i} = -\frac{\partial \epsilon_{\theta}}{\partial k} - B_i(k) \frac{\partial T}{\partial x_i} - 2xk^2 G(k).$$
 (B.2)

We have generalized Phillips' derivation by allowing the mean magnitudes to vary in any arbitrary direction while linearly in the scales considered. The second terms on the left-hand sides correspond to the variation of E(k) and G(k) due to the transfer in physical space by the turbulence itself and, following Phillips, can be neglected in the scales considered;  $\epsilon(k)$  and  $\epsilon_{\theta}(k)$  represent the net rate of spectral energy and mean-square temperature fluctuation transfer, respectively, from wavenumbers smaller than k to wavenumbers larger than k;  $\beta_{ij}(k)$  and  $B_i(k)$  are the spectra of  $b_{ij}$  and  $u_i \theta$ , respectively. Following Phillips, we further consider a statistically stationary state with negligible contribution of the molecular terms and of the Reynolds stresses, both of which are important at larger and smaller wavenumbers, respectively, to obtain the reduced system

$$\frac{\partial}{\partial k} \epsilon(k) = \lambda_i B_i(k) \tag{B.3}$$

$$\frac{\partial}{\partial k} \, \epsilon_{\theta}(k) = -B_i(k) \, \frac{\partial T}{\partial x_i} \,. \tag{B.4}$$

At this point we refer to Weinstock's derivation of  $B_i(k)$ , which we trivially generalize to include variations of T in arbitrary directions thanks to the assumed isotropy. The result is [Weinstock 1978a, Eq. (25) without the factor  $g\alpha$  that we have included in  $\lambda_i$ 

$$B_i(k) = -b \operatorname{Ko}_{\epsilon}(k)^{2/3} \frac{e^{1/2} k^{-2/3}}{k^2 e + 6/5 N^2} \left(\frac{\partial T}{\partial x_i}\right), \quad (B.5)$$

where  $b = (3/2)^{1/2}a$  and the factor a accounts for possible anisotropy effects, and we shall take it to be unity.

When Eq. (B.5) is substituted in Eq. (B.3), one obtains for  $\epsilon(k)$  the following expression

$$\epsilon(k) = \epsilon \left[ 1 + \frac{1}{3} b \text{ Ko} N^2 \epsilon^{-1/3} k_B^{-5/3} e^{-1/2} C(k/k_B) \right]^3$$
(B.6)

where the wavenumber  $k_B$  is defined as

$$k_B = \left(\frac{6}{5}\right)^{1/2} N e^{-1/2} \tag{B.7}$$

and where

$$C(y) = \int_{y}^{\infty} x^{-2/3} (1 + x^2)^{-1} dx.$$
 (B.8)

Here,  $\epsilon = \epsilon(\infty)$ . With this expression for  $\epsilon(k)$  one then resorts to the so-called "local inertiality" hypothesis to write

$$E(k) = \text{Ko}\epsilon(k)^{2/3}k^{-5/3}$$
. (B.9)

Inserting (B.6)-(B.9) into the expression for the turbulent kinetic energy of the subgrid scales, namely,

$$e = \int_{k_m}^{\infty} E(k)dk, \quad k_m = \pi/\Delta, \qquad (B.10)$$

Eq. (16). With the expression for  $c_{\epsilon}$  given by Eq. (20), we finally obtain for C.

$$C_{\epsilon} = c_{\epsilon} S_0^3 \text{ Ko}^{9/2} I_1^3(y_m) y_m [(1+\delta)^{1/2} - 1]^3, \quad (B.11)$$

$$S_0 = b(25/486)^{1/2}$$

$$\delta = \frac{3}{2} I_1^{-2} y_m^{-2/3} \left( \frac{324}{25} b^{-2} \text{ Ko}^{-3} - I_2 \right)$$

$$y_m = \frac{k_m}{k_B} = \left( \frac{5\pi^2}{6} \right)^{1/2} \frac{e^{1/2}}{\Delta N}$$

$$I_n = \int_0^\infty C^n(x) x^{-5/3} dx.$$
(B.13)

The expression for C<sub>i</sub> is only a function of the turbulent kinetic energy through the dimensionless variable  $N\Delta$ /  $e^{1/2}$ . For neutral stratification

$$N \to 0$$
,  $v_m \to \infty$ ,  $C_s \to c_s$ . (B.14)

In the general case, we have found that it is possible to fit the numerical values of  $C_{\epsilon}(e)$  with an expression of the form

$$C_{\epsilon}(e) = c_{\epsilon} \exp(-0.053x^2), \quad x = \frac{N\Delta}{e^{1/2}}.$$
 (B.15)

Next, we obtain an expression for  $\epsilon_{\theta}$ . From Eqs. (B.3)-(B.4), we derive

$$\frac{\partial}{\partial k} \epsilon_{\theta}(k) = -\gamma \frac{\partial}{\partial k} \epsilon(k), \qquad (B.16)$$

where  $\gamma \equiv N^{-2} |\nabla T|^2$ . Upon integration, one gets

$$\epsilon_{\theta}(k) = \epsilon_{\theta} - \gamma [\epsilon(k) - \epsilon].$$
 (B.17)

Substituting (B.17) into the definition of G(k) written assuming the "local inertiality" hypothesis

$$G(k) = Ba\epsilon_{\theta}(k)\epsilon^{-1/3}(k)k^{-5/3},$$
 (B.18)

we can derive an expression for  $\overline{\theta^2}$  from Eq. (19). Using Eqs. (10), one finally gets

$$C_{\theta}(e) = C_{\epsilon}(e)\omega^{-1} \left[ \frac{c_{\theta}}{c_{\epsilon}} - 2\gamma(\omega - 1) \frac{e}{\theta^{2}} \right], \quad (B.19)$$

where

$$\omega = \frac{2}{3} y_m^{2/3} I(y_m) (C_{\epsilon}(e)/c_{\epsilon})^{2/3}$$
 (B.20)

$$I(y_m) = \int_{y_m}^{\infty} x^{-5/3} [1 + \eta C(x)]^{-1} dx \quad (B.21)$$

$$\eta = \frac{5b}{18} \left(\frac{3}{2}\right)^{1/2} \text{Ko}^{3/2} y_m^{-1/3} (C_{\epsilon}(e)/c_{\epsilon})^{-1/3}. \quad (B.22)$$

one can express  $\epsilon$  in terms of e in the form given by It is easy to check that in the neutral case,  $y_m \to \infty$ ,

 $\omega \to 1$ , and thus,  $C_\theta/c_\theta \to C_\epsilon/c_\epsilon$ . We have computed  $\omega$  and found that it can be parameterized as

$$\omega(e) = \exp(-0.053x^2),$$
 (B.23)

where x is defined in Eq. (B.15). Since  $C_{\epsilon}$  has already been parameterized in terms of the kinetic energy by Eq. (B.15), the expression for  $C_{\theta}(e)$  can also be considered given in terms of the energy e and  $\theta^2$ .

#### APPENDIX C

# **Subgrid Scales: The FOC Model**

Here we review some of the FOC models based on Eqs. (6), (7), and (8).

a. The Kolmogoroff (1942)-Prandtl model (1945) (Rodi 1984)

This FOC model can be obtained by taking  $t_1 = t_2 = 0$  in Eq. (7), so that

$$b_{ij} = -2K_m S_{ij}. (C.1)$$

Making use of Eq. (16), one obtains

$$K_m = Ce^{1/2}\Delta, \tag{C.2}$$

where  $C = \frac{2}{3}(1 - \alpha_0)(C_{\epsilon}c_4)^{-1}$ ;  $C_{\epsilon}$  is usually identified with the constant  $c_{\epsilon}$ .

# b. Smagorinsky (1963) and Lilly (1966) extension of the FOC model

Equation (C.2) still expresses  $K_m$  in terms of the kinetic turbulent energy that must be obtained by solving Eq. (6a). A further simplification of the latter equation consists of taking the stationary case and neglecting the third-order moment. This leads to

$$\epsilon = g_i \alpha \overline{u_i \theta} - b_{ij} S_{ij}, \qquad (C.3)$$

which finally yields

$$K_m = (C_S \Delta)^2 S (1 - \sigma_L^{-1} \text{Ri})^{1/2},$$
 (C.4)

where  $C_S$  is the Smagorinsky constant, which in principle is now energy dependent; that is,

$$C_S^2 = C^{3/2} C_{\epsilon}^{-1/2}.$$
 (C.5)

Here, S is the shear,  $S^2 = 2(S_{ij}S_{ij})$ , R is the Richardson number  $Ri = N^2/S^2$ , N is the Brunt-Väisälä frequency,  $N^2 = g_i \alpha \partial T/\partial x_i$ , and  $\sigma_i = K_m/K_h$  is the turbulent Prandtl number. In deriving (C.4) we have introduced a turbulent diffusivity  $K_h$  via

$$\overline{u_i\theta} = -K_h \partial T / \partial x_i \,. \tag{C.6}$$

For neutral stratification, Ri = 0, Eq. (C.4) coincides with the Smagorinsky model, whereas for  $Ri \neq 0$ , it is Lilly's model. It is clear that without further relations, the formula for  $K_m$  is incomplete since the turbulent

Prandtl number  $\sigma_t$ , which in principle is a function of the Richardson number, it not given by the model.

c. The Nieuwstadt (1990) model

This FOC model is derived by taking  $t_1 = t_2 = t_3 = 0$  in Eqs. (7) and (8). One derives

$$K_m = a\Delta e^{1/2}, \quad K_h = b\Delta e^{1/2},$$
 (C.7)

with  $b = (2/3c_6C_\epsilon)$  and  $a = \frac{2}{3}(1 - \alpha_0)(c_4C_\epsilon)^{-1}$ . For unstably stratified flows  $C_\epsilon = c_\epsilon$ , whereas in the case of stably stratified flows,  $C_\epsilon$  is taken in accordance with Deardorff's model (1980), which we have discussed in the Conclusions.

# d. The Mason (1989) model

In his LES work, Mason adopted Eq. (C.4) rewritten as

$$K_m = C_S^2 \Delta^2 S (1 - \beta R_f)^{1/2} (1 + \lambda_0 / \kappa z)^{-2},$$
 (C.8)

where  $R_f$  is the flux Richardson number  $R_f = \sigma_t^{-1}$  Ri,  $\kappa$  is the von Kármán constant, and  $\lambda_0 = C_S \Delta$ . The parameter  $\beta$  is such that when  $R_f < 0$ ,  $\beta = 1$ ; when  $R_f > 0$ ,  $\beta = 3$  and finally, for  $R_f > \beta^{-1}$ ,  $K_m = 0$ . The turbulent diffusivity  $K_h$  is given by  $\sigma_t K_h = K_m$  with the turbulent Prandtl number  $\sigma_t$  assumed to be 1/2. The z dependence in (C.8) assures a smooth joining with the Obhukov similarity law.

# e. The Moeng (1984) and Moeng and Wyngaard (1989) models

In their LES work the authors adopted the original Deardorff (1980) model whereby

$$\epsilon = Ce^{3/2}l^{-1}, K_m = 0.1e^{1/2}l, K_h = (1 + 2l/\Delta)K_m,$$
(C.9)

where  $C = 0.19 + 0.51l/\Delta$ . In (C.9),  $l = \Delta$  for unstable stratification, while  $l = 0.76e^{1/2}N^{-1}$  for stable stratification. In a stably stratified case, Deardorff's expression for  $\epsilon$  can be recast in the form (16) with the result that

$$C_{\epsilon}(e) = c_{\epsilon}^* \left( 1 + \frac{1}{2} x \right), \tag{C.10}$$

where  $c_{\epsilon}^* = 1/2$  and x, is defined by Eq. (23b).

As one can see, Deardorff's  $C_{\epsilon}$  is an *increasing* function of x, whereas the present model predicts a  $C_{\epsilon}$  that decreases with x.

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